Anisole 100-66-3 | DTXSID4041608

Model Performance

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Model	I)ata
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Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 151 °C

Global applicability domain: Inside

Local applicability domain index: 6.78e-01

Confidence level: 7.91e-01

Nearest Neighbors from the Training Set

Image not found

Anisole
Measured: 154

Measured: 154 Predicted: 151 Image not found

1,3,5,7-Cyclooctatetraene

Measured: 141 Predicted: 150 Image not found

Benzyl chloride Measured: 179 Predicted: 162

Image not found

Ethylbenzene Measured: 136 Predicted: 142